

Decay of DNLS breathers through inelastic multiphonon scattering

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We consider the long-time evolution of weakly perturbed discrete nonlinear Schrödinger breathers. While breather growth can occur through nonlinear interaction with one single initial linear mode, breather decay is found to require excitation of at least two independent modes. All growth and decay processes of lowest order are found to disappear for breathers larger than a threshold value.

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The study of intrinsically localized modes in anharmonic lattices, *discrete breathers*, has yielded much attention during the last decade (see e.g. [1,2]). In particular, their existence as time-periodic solutions of nonlinear lattice-equations was proven under quite general conditions [3], and numerical schemes were developed for their explicit calculation [4]. The generality of the concept of discrete breathers, which provide very efficient means to localize energy, has lead to numerous suggestions to its application in contexts where anharmonicity and discreteness are important, e.g. for describing energy and charge transport and storage in biological macromolecules [5]. Recently, discrete breathers have been experimentally observed in coupled optical waveguides [6], in charge-density wave systems [7], in magnetic systems [8], and in arrays of coupled Josephson junctions [9].

Although a discrete breather under quite general conditions is linearly stable [1,3,10] (and thus no perturbations grow exponentially), there are many questions remaining concerning the long-time fate of perturbed breathers. In a previous paper [11], some of these questions were addressed considering a particular model, the discrete nonlinear Schrödinger (DNLS) equation. The interaction between stationary breathers and small perturbations corresponding to time-periodic eigensolutions to the linearized equations of motion around the breather was investigated using a multiscale perturbational approach, and it was found that the nonlinear interaction between the breather and single-mode small-amplitude perturbations could lead to breather *growth* through generation of radiating higher harmonics, but not to breather *decay*. It is the purpose of this Report to extend these results to more general perturbations of stationary DNLS breathers. In particular, we find that while the simplest growth process can be described as an inelastic scattering process with a one-frequency incoming wave and an additional outgoing higher-harmonic wave, the description of a decay process requires *at least two* incoming modes yielding outgoing modes with frequencies being linear combinations of the original ones.

In order to make this Report self-contained, we first recapitulate the main formalism from [11] (to which the reader is referred for details; see also [12] for a similar approach in continuous NLS models). With canonical conjugated variables $\{i\psi_n\}, \{\psi_n^*\}$, the DNLS equation can be derived from the Hamiltonian

$$\mathcal{H}(\{i\psi_n\}, \{\psi_n^*\}) = \sum_n \left(C|\psi_{n+1} - \psi_n|^2 - \frac{1}{2}|\psi_n|^4 \right) \quad (1)$$

as

$$i\dot{\psi}_n = \frac{\partial \mathcal{H}}{\partial \psi_n^*} = -C(\Delta\psi)_n - |\psi_n|^2\psi_n, \quad (2)$$

where Δ is the discrete Laplacian, $(\Delta\psi)_n = \psi_{n+1} + \psi_{n-1} - 2\psi_n$, and we will assume $C > 0$ without loss of generality. In addition to the Hamiltonian (1), a second conserved quantity, the *excitation norm*, is defined as

$$\mathcal{N} = \sum_n |\psi_n|^2. \quad (3)$$

The conservation laws for these two quantities can be expressed in terms of continuity equations, with flux densities for the Hamiltonian and norm given by, respectively,

$$J_{\mathcal{H}} = -2C\text{Re}[\dot{\psi}_{n+1}(\psi_{n+1}^* - \psi_n^*)], \quad (4)$$

$$J_{\mathcal{N}} = 2C\text{Im}[\psi_n^*\psi_{n+1}]. \quad (5)$$

The single-site breather is a localized stationary solution to Eq. (2) of the form $\psi_n(t) = \phi_n(\Lambda)e^{i\Lambda t}$, where $\{\phi_n\}$ is time-independent with a single maximum *at* a lattice site (see e.g. [13,3,14]). It exists for all $\Lambda/C > 0$, and is a ground state solution minimizing the Hamiltonian (1) for a fixed value of the norm (3) (see e.g. [14]). Denoting the values of these quantities for the breather as $\mathcal{H}_\phi(\Lambda) (< 0)$ and $\mathcal{N}_\phi(\Lambda) (> 0)$, respectively, we have:

$$\frac{d\mathcal{N}_\phi}{d\Lambda} = -\frac{1}{\Lambda} \frac{d\mathcal{H}_\phi}{d\Lambda} > 0, \quad (6)$$

proving linear stability of the breather [15] as well as Lyapunov stability for norm-conserving perturbations [14].

To describe the dynamics close to the breather, we introduce the perturbation expansion (cf. [11])

$$\begin{aligned} \psi_n(t) = & \{\phi_n + \lambda\epsilon_n(t) + \lambda^2\eta_n(t) + \lambda^3\xi_n(t) \\ & + \lambda^4\theta_n(t) + \dots\} e^{i\int \Lambda dt}, \end{aligned} \quad (7)$$

where $\epsilon_n(0)$ is the initial small-amplitude perturbation. Substituting into Eq. (2) and identifying coefficients for consecutive powers of the small parameter λ yields for $\lambda^0, \lambda^1, \lambda^2, \lambda^3$, etc:

$$-\Lambda\phi_n + C(\Delta\phi)_n + |\phi_n|^2\phi_n = 0, \quad (8)$$

$$(\mathcal{L}^{(\Lambda)}\epsilon)_n = 0, \quad (9)$$

$$(\mathcal{L}^{(\Lambda)}\eta)_n = -\phi_n^*\epsilon_n^2 - 2\phi_n|\epsilon_n|^2, \quad (10)$$

$$(\mathcal{L}^{(\Lambda)}\xi)_n = -2\phi_n^*\epsilon_n\eta_n - 4\phi_n\text{Re}[\epsilon_n\eta_n^*] - |\epsilon_n|^2\epsilon_n, \quad (11)$$

etc., where $(\mathcal{L}^{(\Lambda)}\epsilon)_n \equiv i\dot{\epsilon}_n + C(\Delta\epsilon)_n + 2|\phi_n|^2\epsilon_n + \phi_n^2\epsilon_n^* - \Lambda\epsilon_n$. The 0th order equation (8) yields the breather shape $\{\phi_n\}$ (which for the single-site breather can be assumed real and positive without loss of generality), the 1st order equation (9) is the linearization of the DNLS equation for small breather perturbations, while the higher order equations describe the long-time dynamics on increasingly longer time-scales.

The linearized solutions are conveniently obtained by substituting $\epsilon_n(t) = \frac{1}{2}a(U_n + W_n)e^{-i\omega t} + \frac{1}{2}a^*(U_n^* - W_n^*)e^{i\omega t}$ into Eq. (9). This yields (for real ϕ_n) an eigenvalue problem of the form $\begin{pmatrix} 0 & \mathcal{L}_0 \\ \mathcal{L}_1 & 0 \end{pmatrix} \begin{pmatrix} \{U_n\} \\ \{W_n\} \end{pmatrix} = \omega \begin{pmatrix} \{U_n\} \\ \{W_n\} \end{pmatrix}$, with Hermitian operators \mathcal{L}_0 and \mathcal{L}_1 defined by (cf. [16])

$$\mathcal{L}_0 W_n \equiv -C(\Delta W)_n - \phi_n^2 W_n + \Lambda W_n, \quad (12)$$

$$\mathcal{L}_1 U_n \equiv -C(\Delta U)_n - 3\phi_n^2 U_n + \Lambda U_n. \quad (13)$$

As the breather is linearly stable for all Λ [15], the eigenvalues ω are real, and the eigenvectors $(\{U_n\}, \{W_n\})$ can be chosen real and normalized. The continuous (phonon) spectrum of extended eigensolutions is obtained for $|n| \rightarrow \infty$ ($\phi_n \rightarrow 0$) yielding two uncoupled equations for the linear combinations $U_n \pm W_n$. Considering without loss of generality only the positive-frequency solutions $U_n + W_n \sim e^{iqn}$ yields the dispersion relation $\omega = \Lambda + 2C(1 - \cos q)$, so that the continuous spectrum for $\omega > 0$ is the interval $\omega \in [\Lambda, \Lambda + 4C]$. Isolated eigenvalues $\omega \neq 0$ outside the continuous spectrum give localized eigensolutions corresponding to breather internal modes [17,18]: one spatially symmetric, 'breathing', mode exists for $0 < \Lambda/C \lesssim 1.7$, and one antisymmetric, 'translational' or 'pinning' mode for $0 < \Lambda/C \lesssim 1.1$. (The variation of their frequencies with Λ/C was shown in Fig. 1 of [11]). Finally, there are also the zero-frequency solutions to Eq. (9), obtained from the ansatz $\epsilon_n = U_n + iW_n$. They can be written as a superposition of two fundamental modes: the 'phase mode' [19] $W_n = \phi_n$ describing a rotation of the overall phase of the breather, and the 'growth mode' [19] $U_n = \partial\phi_n/\partial\Lambda$ (yielding $\epsilon_n = \partial\phi_n/\partial\Lambda + i\phi_n t$) describing a change of breather frequency.

This set of eigenvectors (including the zero-frequency modes) forms a basis for the space of solutions to Eq. (9), in which an arbitrary initial perturbation can be expanded. Eigenvectors $(\{U_n^{(i)}\}, \{W_n^{(i)}\})$ with different (real) eigenvalues $\omega^{(i)}$ fulfill the orthogonality relations

$$(\omega^{(i)} - \omega^{(j)}) \sum_n (U_n^{(i)} W_n^{(j)*} + W_n^{(i)} U_n^{(j)*}) = 0, \quad (14)$$

and, with the 'pseudoscalar' product defined from (14), the only nonzero product involving the zero-frequency modes is their cross-product [15]:

$$\sum_n \phi_n \frac{\partial\phi_n}{\partial\Lambda} = \frac{1}{2} \frac{d\mathcal{N}_\phi}{d\Lambda} > 0. \quad (15)$$

Let us now discuss the long-time effects of a small initial breather perturbation, expanded in the above basis. The second-order correction to the linearized dynamics is given by the inhomogeneous Eq. (10). As its right-hand side is quadratic in ϵ , it describes fundamental scattering processes involving at most two modes: assuming the initial perturbation $\epsilon_n(0)$ to consist of a set of modes with frequencies $\{\omega^{(i)}\}$, the right-hand side will contain the frequencies $\{2\omega^{(i)}\}$, $\{\omega^{(i)} + \omega^{(j)}\}$, $\{|\omega^{(i)} - \omega^{(j)}|\}$ and 0. Thus, it acts as a multi-periodic force localized at the breather region (since all terms are multiplied by ϕ_n), and resonances with solutions to the homogeneous Eq. (9) typically yields a response for $\{\eta_n\}$ which either diverges in time (resonance with discrete spectrum) or is spatially unbounded (resonance with continuous part).

In a standard way, the divergent parts can be removed by allowing for a slow, adiabatic time-evolution of the breather parameters. Similarly as in [11], where the case of single-mode initial perturbations was analyzed in detail, the divergence due to overlap between the static part of the right-hand side of (10) and the zero-frequency modes can be shown to be equivalent to a time-independent shift of the breather frequency Λ . Writing $\Lambda = \Lambda_0 + \lambda^2\Lambda_2$, where Λ_0 is the unperturbed breather frequency, the second-order shift Λ_2 will be the sum of the shifts resulting from the individual modes contained in $\epsilon_n(0)$. The latter was calculated in [11] (cf. Eq. (31)), and generalizes for the multimode case to

$$\Lambda_2 = \frac{1}{\frac{d\mathcal{N}_\phi}{d\Lambda}} \sum_n \phi_n \frac{\partial\phi_n}{\partial\Lambda} \sum_i |a^{(i)}|^2 (3(U_n^{(i)})^2 + (W_n^{(i)})^2),$$

where $a^{(i)}$ is the initial amplitude for the mode $(\{U_n^{(i)}\}, \{W_n^{(i)}\})$ with frequency $\omega^{(i)}$. In general, Λ_2 can be either positive or negative, depending on the detailed spatial structure of the excited eigenmodes.

The spatially unbounded response resulting from resonances between the oscillating part of the right-hand side of (10) and phonon modes physically corresponds to emission of radiation from the breather region for each oscillation frequency belonging to the continuous spectrum of (9). The strength of the radiation fields can be calculated as illustrated in [11] for second-harmonic ($2\omega^{(i)}$) resonances (cf. Eq. (34) and the following discussion); here we give the corresponding results for two-mode ($\omega^{(i)} \pm \omega^{(j)} \equiv \omega^{(\pm)}$) resonances (assuming $\omega^{(i)} > \omega^{(j)}$ without loss of generality). Writing the corresponding responses as $\eta_n^{(\pm)} = \frac{1}{2}A_{ij}^{(\pm)}(u_n^{(\pm)} + w_n^{(\pm)})e^{-i\omega^{(\pm)}t} + \frac{1}{2}A_{ij}^{(\pm)*}(u_n^{(\pm)*} - w_n^{(\pm)*})e^{i\omega^{(\pm)}t}$, with $A_{ij}^{(+)} = a^{(i)}a^{(j)}$

and $A_{ij}^{(-)} = a^{(i)}a^{(j)*}$, the functions $u_n^{(\pm)}$ and $w_n^{(\pm)}$ are determined by $\begin{pmatrix} -\omega^{(\pm)} & \mathcal{L}_0 \\ \mathcal{L}_1 & -\omega^{(\pm)} \end{pmatrix} \begin{pmatrix} \{u_n^{(\pm)}\} \\ \{w_n^{(\pm)}\} \end{pmatrix} = \frac{\phi_n}{2} \begin{pmatrix} \{W_n^{(i)}U_n^{(j)} \pm U_n^{(i)}W_n^{(j)}\} \\ \{3U_n^{(i)}U_n^{(j)} \mp W_n^{(i)}W_n^{(j)}\} \end{pmatrix}$. When $\omega^{(\pm)}$ belongs to the phonon band, the radiation field strength will be proportional to the overlap between this right-hand-side and the corresponding continuous spectrum eigenvector $(\{U_n^{(\pm)}\}, \{W_n^{(\pm)}\})$, which using (14) is obtained as

$$c^{(\pm)} = \frac{1}{2} \sum_n \phi_n \left[W_n^{(\pm)} (W_n^{(i)}U_n^{(j)} \pm U_n^{(i)}W_n^{(j)}) + U_n^{(\pm)} (3U_n^{(i)}U_n^{(j)} \mp W_n^{(i)}W_n^{(j)}) \right]. \quad (16)$$

Far away from the breather, the radiation field should correspond to two identical outgoing propagating linear waves, yielding the boundary conditions $u_n^{(\pm)}, w_n^{(\pm)} \rightarrow r^{(\pm)}e^{\pm iq^{(\pm)}n}, n \rightarrow \pm\infty$ where $r^{(\pm)} \sim c^{(\pm)}$ and $q^{(\pm)} = \arccos\left(1 - \frac{\omega^{(\pm)} - \Lambda}{2C}\right)$ from the linear dispersion relation.

Let us now discuss the consequences of the second-order radiation arising from the two-mode-interaction for the breather itself. Assume for simplicity that only two modes with frequencies $\omega^{(1)}$ and $\omega^{(2)}$ ($\omega^{(1)} > \omega^{(2)}$) are initially excited (the presence of other modes will contribute to orders 3 and higher), and that both modes belong to the continuous spectrum (the case of internal mode excitation requires some modification, see [11], Sec. IIIC). Far away from the breather, we assume a stationary regime which, in the most general case when $2\omega^{(1)}, 2\omega^{(2)}, \omega^{(+)} \text{ and } \omega^{(-)}$ all belong to the phonon spectrum, corresponds to the boundary conditions at $n \rightarrow \pm\infty$:

$$\begin{aligned} \psi_n \rightarrow & e^{i\Lambda t} \left[a^{(1)} (e^{\mp iq^{(1)}n} + r^{(1)}e^{\pm iq^{(1)}n}) e^{-i\omega^{(1)}t} \right. \\ & + a^{(2)} (e^{\mp iq^{(2)}n} + r^{(2)}e^{\pm iq^{(2)}n}) e^{-i\omega^{(2)}t} \\ & + (a^{(1)})^2 r_2^{(1)} e^{i(\pm q_2^{(1)}n - 2\omega^{(1)}t)} \\ & + (a^{(2)})^2 r_2^{(2)} e^{i(\pm q_2^{(2)}n - 2\omega^{(2)}t)} \\ & + a^{(1)} a^{(2)} r^{(+)} e^{i(\pm q^{(+)}n - \omega^{(+)}t)} \\ & \left. + a^{(1)} (a^{(2)})^* r^{(-)} e^{i(\pm q^{(-)}n - \omega^{(-)}t)} \right]. \quad (17) \end{aligned}$$

Note that in general, the stationary amplitudes for the outgoing fundamental waves will differ from those of the incoming (i.e., $r^{(1)}, r^{(2)} \neq 1$); this is a consequence of resonances at the frequencies $\omega^{(1)}$ and $\omega^{(2)}$ in Eq. (11) for the third-order field ξ_n . For a general multimode perturbation, it is seen from (11) that this correction takes the form $r^{(i)} = 1 + \sum_j \alpha_{ij} |a^{(j)}|^2$, where the sum goes over all initially excited modes (here $j = 1, 2$).

We then consider the conservation laws for the total norm and Hamiltonian, respectively, contained in some region around the breather. Assuming the breather frequency Λ to be the only time-dependent parameter in

the stationary regime we can, similarly as in Ref. [11], Sec. IV, write the time-averaged balance equations as

$$\frac{d\langle \mathcal{N} \rangle_t}{dt} = \frac{d\mathcal{N}_\phi}{d\Lambda} \dot{\Lambda} = \langle J_{\mathcal{N}}(-\infty) \rangle_t - \langle J_{\mathcal{N}}(+\infty) \rangle_t, \quad (18)$$

$$\frac{d\langle \mathcal{H} \rangle_t}{dt} = \frac{d\mathcal{H}_\phi}{d\Lambda} \dot{\Lambda} = \langle J_{\mathcal{H}}(-\infty) \rangle_t - \langle J_{\mathcal{H}}(+\infty) \rangle_t. \quad (19)$$

As the time-average of the flux densities $J_{\mathcal{N}}$ and $J_{\mathcal{H}}$ are additive quantities for small-amplitude plane waves of the form $\psi_n = Ae^{i(Qn - \Omega t)}$, the right-hand sides are readily obtained from (17) using the general expressions $J_{\mathcal{N}} = 2|A|^2 C \sin Q$ and $J_{\mathcal{H}} = \Omega J_{\mathcal{N}}$ for the individual waves resulting from (4)-(5). Combining Eqs. (18)-(19) and using (6) yields the time-derivative of the breather frequency to order 4 in the mode amplitudes $a^{(1)}, a^{(2)}$ as:

$$\begin{aligned} \dot{\Lambda} = & \frac{4C}{\frac{d\mathcal{N}_\phi}{d\Lambda}} \left[|a^{(1)}|^4 |r_2^{(1)}|^2 \sin q_2^{(1)} \right. \\ & + |a^{(2)}|^4 \left(\frac{2\omega^{(2)}}{\omega^{(1)}} - 1 \right) |r_2^{(2)}|^2 \sin q_2^{(2)} \\ & + |a^{(1)}|^2 |a^{(2)}|^2 \frac{\omega^{(2)}}{\omega^{(1)}} \left(|r^{(+)}|^2 \sin q^{(+)} - |r^{(-)}|^2 \sin q^{(-)} \right) \\ & \left. + |a^{(2)}|^2 \left(1 - \frac{\omega^{(2)}}{\omega^{(1)}} \right) \left(1 - |r^{(2)}|^2 \right) \sin q^{(2)} \right]. \quad (20) \end{aligned}$$

For a single-mode initial excitation, $a^{(2)} = 0$ and only the first, positive term of the right-hand side remains, so that we recover the result (Eq. (55) in [11]) that the generation of second-harmonic radiation always leads to breather *growth*. However, in the two-mode case, the expression (20) is in general not sign-definite, and in particular the contribution from the frequency $\omega^{(-)}$ is always negative. It is therefore natural to associate this radiation with the *fundamental lowest-order mechanism for breather decay*. This can be seen as a consequence of the Hamiltonian flux density being proportional to the frequency for plane waves. Thus the scattering towards the lower frequency $\omega^{(-)}$ should yield a net flow of negative Hamiltonian energy out from the breather region, to which the breather adapts by decreasing its frequency and amplitude according to (6). On the other hand, the generation of radiation with the higher frequency $\omega^{(+)}$ should analogously contribute to breather growth, as for the second-harmonic case. (See also [20] for a similar explanation of breather decay in a Klein-Gordon model resulting from a resonance in the linearized equations.)

It is important to note, that when $\omega^{(1)}$ and $\omega^{(2)}$ are phonon modes, they fulfill $\Lambda \leq \omega^{(1)}, \omega^{(2)} \leq \Lambda + 4C$, so that we have $0 \leq \omega^{(1)} - \omega^{(2)} \leq 4C$ and $2\Lambda \leq 2\omega^{(1)}, 2\omega^{(2)}, \omega^{(1)} + \omega^{(2)} \leq 2\Lambda + 8C$. Thus, we see that second order radiation can only be generated if the breather frequency fulfills $0 < \Lambda \leq 4C$, since for $\Lambda > 4C$ the frequency $\omega^{(-)}$ is always below the phonon band, while $2\omega^{(1)}, 2\omega^{(2)}$ and $\omega^{(+)}$ are always above. Therefore, when

$\Lambda > 4C$ all terms in the right-hand side of Eq. (20) necessarily vanish, and *all growth and decay processes of lowest order disappear*. Numerically, we found [11] that this corresponds to breathers with central-site intensity $|\psi_{n_0}|^2 \gtrsim 5.65$. Therefore, these large-amplitude breathers are particularly stable, since all possible growth and decay processes result from third- and higher-order radiation processes so that the rate of their growth/decay must be at least of order 6 in the initial mode amplitudes.

To illustrate the fundamental lowest-order decay mechanism, we consider the 'pure' case when $\omega^{(-)}$ belongs to the phonon spectrum, while $2\omega^{(1)}, 2\omega^{(2)}$, and $\omega^{(+)}$ are outside. Thus, we have $r_2^{(1)} = r_2^{(2)} = r^{(+)} = 0$, and only the last two terms in Eq. (20) are nonzero. We note that if $|r^{(2)}| < 1$, the last term will be positive, and we can therefore in general not conclude that Λ must be negative. The reason is, that although the scattering towards the lower frequency $\omega^{(-)}$ from either of the two frequencies $\omega^{(1)}$ or $\omega^{(2)}$ considered independently would yield a net outflow of negative Hamiltonian energy from the breather region and thereby breather decay, there will also be a contribution from the mixing between the $\omega^{(1)}$ and $\omega^{(2)}$ modes arising from the third order equation (11). This contribution would yield a net outflow of positive Hamiltonian energy if $|r^{(2)}| < 1$ and $|r^{(1)}| > 1$, and could therefore contribute to breather growth. However, extensive numerical simulations for different Λ , $\omega^{(1)}$ and $\omega^{(2)}$ belonging to this region of 'pure' $\omega^{(-)}$ -scattering have always shown that the net result is a linear *decrease* of the breather frequency, and therefore we believe it justified to identify this two-wave scattering as the fundamental lowest-order breather decay mechanism (Fig. 1).

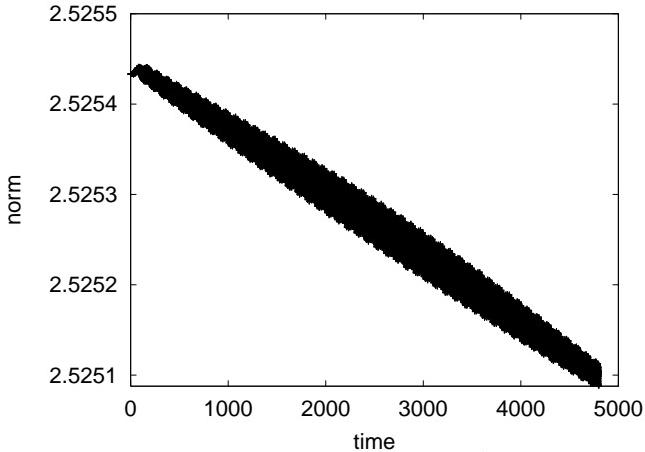


FIG. 1. Time evolution of the total norm \mathcal{N} contained in a region of 120 sites around a breather with frequency $\Lambda = 0.45$, perturbed along two eigenmodes with frequencies $\omega^{(1)} \approx 3.00$ and $\omega^{(2)} \approx 2.47$, respectively ($C = 1$).

In conclusion, we found that while in the DNLS model breather growth can result through interaction between the breather and single-mode initial perturbations, the description of breather decay requires simultaneous excitation of at least two independent linear modes. This

confirms numerical results in Ref. [11] (Figs. 5 and 6), showing breather decay also from initially single-mode perturbations with larger amplitude, as more frequencies became gradually excited e.g. through oscillatory wave instabilities [21]. We believe that our approach could be useful to understand the properties of the stationary intensity probability distribution function in the 'negative temperature'-regime of the DNLS model [22], where persistent localized breathers were found, weakly interacting with small amplitude radiation. Finally, we remark that the DNLS model is nongeneric among Hamiltonian lattice models as it has two conserved quantities, and the DNLS breather has only one fundamental frequency with no harmonics. Thus, our approach cannot immediately be extended to other models exhibiting breathers such as Fermi-Pasta-Ulam or Klein-Gordon lattices. However, as for the latter the DNLS equation is known (see e.g. [21]) to describe the small-amplitude dynamics for small inter-site coupling, we believe that the breather growth and decay mechanisms described here are relevant also in these systems. This will be investigated in future work.

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